Coherence in the Two Kondo Impurity Problem

Lijun Zhu and C. M. Varma

Department of Physics and Astronomy, University of California, Riverside, CA 92521

We show through a perturbative and an exact calculation using Wilson's renormalization methods that in the problem of two interacting Kondo impurities, on-site potential scattering generates a quantum-tunneling between the two impurities through a marginally relevant operator. The magnitude of this tunneling V_{12} depends on the spin-correlation between the two impurities. For exchange interactions between the moments comparable to the Kondo energy T_K, V_{12} is typically much larger than T_K. This implies that the heavy-fermion mass in this interesting range is determined by V_{12} rather than T_K. The importance of these results for experiments in coupled Kondo dots is also pointed out.

The two Kondo impurity problem has been of interest because it presents the competition between mutual interactions of local moments and the Kondo renormalization of the moments to singlet states in a soluble way. An aspect of the problem which has received no attention hitherto is the the low-energy transfer Hamiltonian of quasi-particles between the two impurity sites. In the quasi-particle problem for a lattice, this sets the scale for the heavy-fermion bandwidth. The issue is also directly posed in a recent ingenious realization of the two Kondo impurity problem using coupled quantum dots [1].

The two Kondo impurity problem was solved by numerical renormalization group method (NRG) for a particle-hole symmetric model obtained by ignoring potential scattering [2], and was subsequently studied by conformal field theory [3], bosonization[4] and other methods[5]. In the single Kondo impurity problem, potential scattering merely shifts the Kondo resonance with respect to the chemical potential in accordance with Friedel sum-rule. The sum of the phase shifts in the even and the odd parity channels for the two Kondo impurity problem is fixed by the Friedel sum-rule to be π. Without potential scattering the phase shift in both the even and the odd parity channels is $\pi/2$ when the fixed point is the Kondo fixed point. Consequently, there is no splitting of the even-odd resonances or equivalently, no *direct* hopping of the quasi-particles between the two impurity sites. In this case there is a quantum critical point (QCP) separating the Kondo singlet regime of the impurities from the inter-impurity singlet regime [2].

Affleck and Ludwig [3] pointed out that the QCP is changed to a crossover by the potential scattering only when the exchange scattering at the local moments transfers conduction electron from one impurity to the other. In this paper, we first explain the Affleck-Ludwig result by a simple perturbative calculation. We then obtain the new result that in such a case an even-odd splitting of the resonances is generated which depends on the spin correlations. We then present [6] exact results of a Wilson's NRG calculation to reinforce and quantify these conclusions by deriving the low energy Hamiltonian. These also serve to give the crossover scale of the QCP. The relation of the coherence scale to the bare parameters of the problem and to the generated spin-correlations is explicitly

calculated. These results are of fundamental importance to the problem of the heavy-fermion state.

The interactions between the free electrons and the local moments in the two Kondo impurity problem are [2, 3]

$$
\begin{aligned}
H_{\text{imp}} &= \frac{J_+}{2}\left(\psi_1^\dagger\vec{\sigma}\psi_1 + \psi_2^\dagger\vec{\sigma}\psi_2\right)\cdot(\mathbf{S}_1+\mathbf{S}_2) \\
&+ \frac{J_m}{2}\left(\psi_1^\dagger\vec{\sigma}\psi_1 - \psi_2^\dagger\vec{\sigma}\psi_2\right)\cdot(\mathbf{S}_1-\mathbf{S}_2) \\
&+ \frac{J_-}{2}\left(\psi_1^\dagger\vec{\sigma}\psi_2 + \psi_2^\dagger\vec{\sigma}\psi_1\right)\cdot(\mathbf{S}_1+\mathbf{S}_2) \\
&+ K\mathbf{S}_1\cdot\mathbf{S}_2 + \sum_\sigma V\left(\psi_{1\sigma}^\dagger\psi_{1\sigma}+\psi_{2\sigma}^\dagger\psi_{2\sigma}\right). \quad (1)
\end{aligned}
$$

Here $\mathbf{S}_1$ and $\mathbf{S}_2$ represent two $S=1/2$ Kondo impurities sitting at two lattice sites. $\psi_{1(2)}=\sum_\mathbf{k}\psi_{1(2),k}$; $\psi_{1(2),k}$ are annihilation operators for conduction electrons in spherical waves about the impurity 1 and 2 respectively. $\vec{\sigma}$ are Pauli matrices. J's are the exchange coupling between the local moments and the conduction electrons. V gives the potential scattering; the maximum magnitude of V deduced from the Anderson Hamiltonian is $|J|/4$[7]. It is convenient to choose certain J_m so that the generated RKKY interaction is 0 while introducing such an interaction K explicitly[2, 8]. For the NRG calculation, the representation in terms of even (e) and odd (o) parities of the conduction electron states is more convenient. The latter are obtained by $\psi_{e(o),k}=(\psi_{1,k}\pm\psi_{2,k})/\sqrt{2}$ while $J_{e,o}=J_+\pm J_-$.

Note that in Eq.(1) the only connection between the impurity states is through J_-. (The direct hopping of the impurity orbitals from one impurity site to the other is much much smaller than V, $J's$ or the single-impurity Kondo temperature T_K for rare-earth or actinide moments.) This alone (i.e. with $V=0$) is insufficient for quasi-particle hopping between sites 1 and 2. This can be motivated through a perturbative calculation by the diagrams in Fig.(1).

The vertex can be in general separated as a vector and a scalar part: $\Gamma_{12}=\Gamma_{S,12}\delta_{\alpha\alpha'}+\Gamma_{V,12}\vec{\sigma}_{\alpha\alpha'}\cdot\mathbf{S}$. Here $\mathbf{S}=\mathbf{S}_1+\mathbf{S}_2$. The scalar part, $\Gamma_{S,12}$, is an effective potential scattering electrons between sites 1 and 2. First we consider the limit when two impurities are locked into either a singlet or a triplet states, $S=0$, or 1. The bare
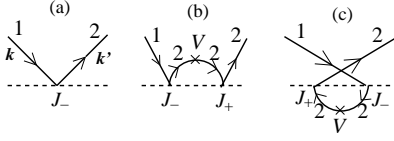
FIG. 1: Vertices diagrams for the two Kondo impurity problem. (a) shows a bare vertex of J_- while (b) and (c) show leading corrections to J_- in particle-particle and particle-hole channels, respectively, which contribute a potential scattering $V_{12}\psi_2^\dagger\psi_1$. Solid and dashed lines represent the propagators of the conduction electrons and the two impurities with a total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$, respectively.

vertex [cf. Fig. 1(a)] is $\Gamma_{V,12}^{(0)} = J_-$. This is corrected by Fig. 1(b) and Fig. 1(c) in next leading order. They exactly cancel if the intermediate particle-line in (b) and hole-line in (c) have the same spectra, i.e. at $V = 0$, or particle-hole symmetry. For $V \neq 0$, the generated vertex (including similar diagrams with ψ_{1k} as the intermediate state) is:

$$\Gamma_{S,12} = \rho^2 \frac{S(S+1)}{2} J_+ J_- (cV),\qquad(2)$$

where ρ is the density of state of conduction electrons at the chemical potential, S is the total spin of the two impurities and c is a dimensionless constant of $O(1)$. Such a term in two Kondo impurity problem generates the new effect, a splitting between even and odd resonances,

$$V_{12}\psi_1^\dagger\psi_2 + h.c. = V_{12}(\psi_e^\dagger\psi_e - \psi_o^\dagger\psi_o).\qquad(3)$$

V_{12} also depends on the spin-states of the two impurities; this is seen from the fact that $V_{12} = V_e - V_o$ while the effective potential scattering including Fig. 1(b-c) is $V_e\psi_e^\dagger\psi_e + V_o\psi_o^\dagger\psi_o$

$$V_{e,o} = V - \frac{S(S+1)}{4} cV\rho^2 (J_+^2 + J_-^2 \pm 2J_+J_-)\qquad(4)$$

When $K \to -\infty$, $S = 1$; then

$$V_{12} \propto V(\rho J_-)(\rho J_+).\qquad(5)$$

However, when $K \to \infty$, $S = 0$, the contribution to the splitting due to V vanishes. In between these limits, there are mixing terms between the triplet and singlet states of two impurities, so that the results depend on the spin-correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$. For the general case and because at least one of the two vertices in Fig.(1), J_+, has singular renormalizations, complete answers can only be obtained by exact methods, for example, Wilson's NRG method[9].

In NRG, the conduction electron band is discretized on a logarithmic grid into a semi-infinite chain with only nearest-neighbor hopping terms (here we have two chains corresponding to even and odd parity degrees of freedom), while the model can be solved recursively by a sequence of H_N's.

$$H_{N+1} = \Lambda^{1/2} H_N + \sum_{p=e,o;\sigma} [f_{pN\sigma}^\dagger f_{p(N+1)\sigma} + \text{H.c.}],\qquad(6)$$

where Λ is the discretization energy scale. The impurities only interact with the first site ($f_{p0\sigma}$) through the Hamiltonian H_0. From the change of spectra with iteration, the fixed points and the dimensions of operators about them are determined.

For $V = 0$, two distinct spectra are identified for large iterations with the tuning of K [2]. When K is large and ferromagnetic, the spectra can be fitted with the effective Hamiltonian

$$H_N = H_N^* + H_{ir},\qquad(7)$$

where the fixed-point Hamiltonians H_N^* in even/odd iterations are the same as those of free-electrons in odd/even iterations, reflecting the $\pi/2$ phase shift in both parity channels and the formation of Kondo resonances. Both resonances develop at the chemical potential, as shown in Fig.(2a). H_{ir} contains terms such as $t_p f_{0p}^\dagger f_{1p} + H.c.$ which vanish at $N \to \infty$ as $\Lambda^{-(N-1)/2}$ reflecting the irrelevant nature. (t_p and other leading irrelevant parameters serve to determine T_K). When K is large and antiferromagnetic, the two impurities form a spin-singlet; the eigenvalues of the actual Hamiltonian do not show the even/odd interchange, reflecting 0 or π (for odd and even parity channels, respectively) asymptotic phase shifts. Near the QCP at $K_c \approx 2.4 T_K^0$, singular fermi-liquid behavior, studied in detail earlier[2, 3] ensues.
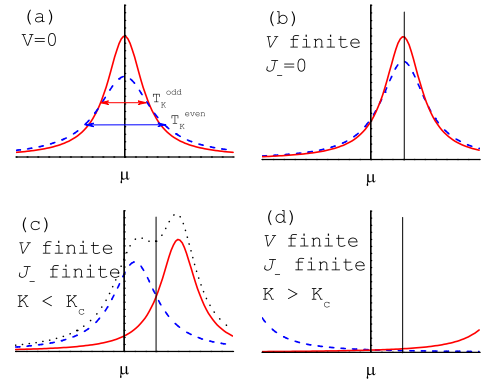

FIG. 2: Spectra for the two Kondo impurity model. The location of the resonance with respect to the chemical potential is determined from the fixed point Hamiltonian and the width from the leading irrelevant operators. (a) shows the particle-hole symmetric case; Kondo resonances of both even and odd parities appear at the chemical potential. (b) for $J_- = 0$ while finite potential scattering V breaks the particle-hole symmetry in each channel; both resonances appear at the same energy but tuned away from the chemical potential. (c) for both finite V and J_- while $K < K_c$; the even and odd resonances split. For (d), when K is bigger than the crossover scale K_c, although the splitting increases, the resonance peaks fall out of the band, reflecting the disappearance of the Kondo effect.

We find in accordance with the perturbative calculation above that the fermi-liquid behavior on either side

and the singular fermi-liquid behavior near the QCP continues for $V \neq 0$, $J_- = 0$ but with equal additional phase shift in both parities so that the asymptotic eigenvalues are given by

$$\sum_p V_p^* f_{0p}^\dagger f_{0p}, \tag{8}$$

with $V_e^* = V_o^*$. This has a scaling dimension 0 and appears as a marginally relevant operator at the two strong-coupling fixed points as well as at the QCP. The conservation of *axial charge* [2, 3] continues to give relation between the coefficients for the irrelevant operators and they diverge in the same manner as at $V = 0$ near the QCP. When $J_- = 0$, the two impurities become effectively two non-interacting Kondo scatters. For each channel, a potential scattering induced phase shift $\delta_v = -\tan^{-1}(\pi\rho_0 V)$ appears in addition to the $\pi/2$ phase shift, as in single Kondo impurity problem[10]. Here, $\delta_e = \delta_o$, two Kondo peaks in local density of states coincide with each other while they are shifted away from the chemical potential [see Fig.(2b)].

It is natural to represent the eigenvalues in the even and odd parity channels in terms of the phase-shifts δ_e and δ_o in these channels, which can obtained from the eigenvalues of the fixed-point Hamiltonian, denoted as ω_{pj}^* for j-th excitation level with p-parity. For free electrons(with vanishing V and J's), the eigenvalues (η_j^*) can be easily obtained numerically for a given Λ. Their values at $N \to \infty$ limit are approximately

$$N \text{ odd:} \quad \eta_j^* = \text{sgn}(j)\Lambda^{|j|-1}, j = \pm 1, \ldots, \pm\frac{1}{2}(N+1),$$

$$N \text{ even:} \quad \hat{\eta}_j^* = \text{sgn}(j)\Lambda^{|j|-1/2}, j = 0, \pm 1, \ldots, \pm\frac{1}{2}N, \tag{9}$$

for $1 \ll |j| \ll N/2$. With interactions, the eigenvalues(ω_j^*) can be associated with η_j^* by a phase-shift factor. Quite generally,

$$\omega_{pj}^* = \Lambda^{-\text{sgn}(\eta_{pj}^*)\delta_p/\pi}\eta_{pj}^*. \tag{10}$$

For instance, at the strong-coupling Kondo fixed point, $\hat{\omega}_j^*$ at even iterations $(\Lambda^{j-1/2}\Lambda^{-1/2})$ are the same as η_j^* in odd iterations, corresponding to a phase shift $\delta_p = \pi/2$. One can then calculate the phase shifts from the numerical data following Eq.(10). The principal results of this paper is the evaluation of δ_e, δ_o and its dependence on K/T_K^0 from which the variation of the coherence scale is determined. These results are displayed in Fig. (3).

In the particle-hole symmetric case ($V = 0$), $\delta_e = \delta_o = \pi/2$ in the Kondo-resonance fixed point, but $\delta_e = \pi$ and $\delta_o = 0$ in the inter-impurity spin-singlet fixed point. The latter merely reflects the fact that in the inter-impurity spin-singlet state, the even parity channel is fully occupied and the odd parity channel is completely empty. An abrupt change of the phase shift happens at the critical point, $K_c \approx 2.4 T_K^0$, where $T_K^0 \approx 1.4 \times 10^{-4}D$, is the single-impurity Kondo temperature (for $J/D = 0.125$). J_- is then irrelevant. When $V \neq 0$ but $J_- = 0$, δ_e
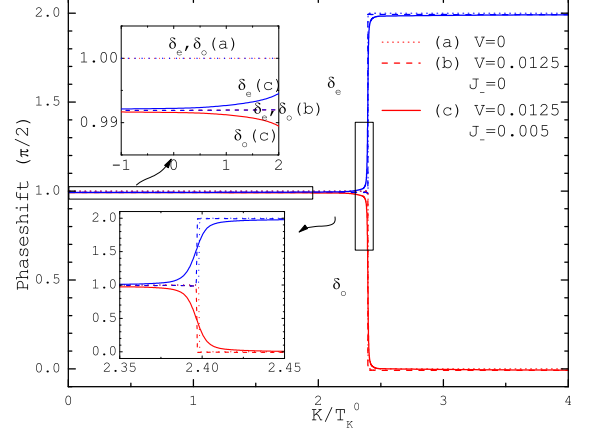

FIG. 3: Phase shifts as functions of K. (a)-(c) show the cases when $V = 0$, $J_- = 0.005$; $V = 0.0125$, $J_- = 0$; and $V = 0.0125$, $J_- = 0.005$, respectively. J_+ is chosen as 0.125.

and δ_o of two phases are shifted equally from $\pi/2$ and π or 0, respectively. They still behave as two independent Kondo impurities; each gains additional δ_v from the potential scattering term. With both finite V and J_-, one can observe two features. 1) the phase shift changes smoothly at a critical value for $K_c(V)$, which smears out the critical point. K_c is a function of V since the potential scattering term renormalizes the Kondo coupling (see perturbative calculation above) thus changing the Kondo temperature. 2) even and odd phase shifts are different while their summation remains $\delta_e + \delta_o = \pi + 2\delta_v$, where δ_v can be associated with its counterpart in one Kondo impurity problem. In this case, although the axial charge in each channel is not separately conserved, their summation is. J_- is a relevant operator removing the critical point if particle-hole symmetry is absent, $V \neq 0$.

Given the phase shifts the potential scattering parameter in the asymptotic Hamiltonian which is a marginal operator are determined through $\delta_{e,o} = -\tan^{-1}(\pi\rho V_{e,o}^*)$,

$$(V_e^* - V_o^*)(f_{e0}^\dagger f_{e0} - f_{o0}^\dagger f_{o0}), \tag{11}$$

which is the coherence operator in effective Hamiltonian

$$H_{coh}^* = V_{12}(\psi_1^\dagger \psi_2 + H.c.), \tag{12}$$

where $V_{12} = D(V_e^* - V_o^*)(1 + \Lambda^{-1})/2$, i.e, V_{12} in Eq.(3) for $\Lambda = 1$.

The dependence on the coherence scale V_{12} on various parameters is shown in Figs.(4,5). V_{12} shows a linear relation with V and J_- for a whole range of K, as shown in Fig.(5a-b). This is in agreement with the perturbation results in $K \to -\infty$ limit, while as expected its dependence on J_+ for a general K is not. The critical point becomes a crossover, as the degeneracy of the singlet and triplet parts of the Hamiltonian is lifted. Close to the
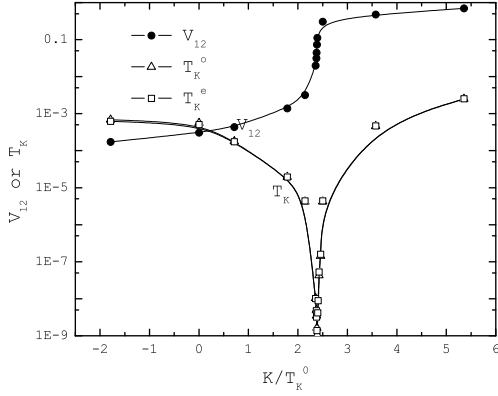
FIG. 4: The dependence of V_{12} and the Kondo temperature T_K (both in unit of the bandwidth W) on the RKKY coupling constant K. Other parameters are fixed as $J_+ = 0.125$, $J_- = 0.005$ and $V = 0.0125$.
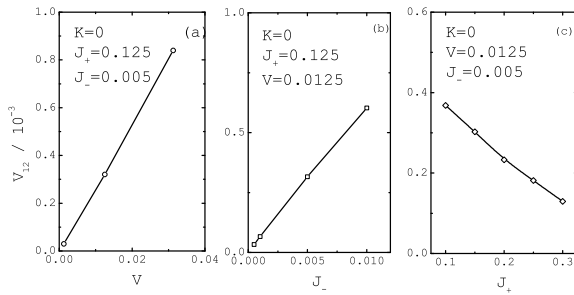

FIG. 5: The dependence of the coherence scale V_{12} on various parameters: a) V; b) J_-; c) J_+ when $K = 0$.

crossover, although V_{12} increases uniformly, the Kondo resonances themselves disappear [cf. Fig.(4)].

Our most important new physical results come from the magnitude of V_{12} and its dependence on K/T_K^0. In the particle-hole symmetric case, such a term vanishes: the quasi-particle does not hop *directly* between the two

sites. (The analog of this effect in the periodic Anderson lattice model, is that the chemical potential falls within the hybridization gap for the particle-hole symmetric case and the system is an insulator [11]). A finite V_{12} has important implications for the heavy-fermion lattice. Heavy-fermion bands have been derived in a variety of ways, all of which have the same physics: constrained hybridization of a periodic array of local orbitals with a wide conduction band with a matrix element of the order of the single Kondo impurity resonance width, i.e., the Kondo temperature. The heavy-fermion bandwidth in such calculations is therefore of $O(T_K)$. However even for $T_K \to 0$, V_{12} gives the order of magnitude of the splitting of the heavy fermion band at the zone-center and the zone-boundary. Therefore, if the lattice problem is solved by a self-consistent two Kondo impurity problem with a cluster generalization of dynamical mean-field theory, the effective bandwidth is then to be determined including both the parameter T_K as well as V_{12}. It is therefore important to consider the relative magnitude of these two parameters. The interesting range for heavy-fermion compounds is for antiferromagnetic coupling K/T_K^0 of $O(1)$. In this range for the typical parameters shown in Fig.(4), V_{12} is more than an order of magnitude larger than T_K. The conclusion then is that the effect of V_{12} dominates in the low energy mass and thermodynamic and transport properties. It is interesting that this term already includes renormalizations due to spin-correlations, which are further augmented by Landau-parameters.

In the regime of large K/T_K^0, the T_K given in Fig.(4) reflects only that the spectral weight at the chemical potential is only of $O(T_K/V_{12}^2)$. This reflects the disappearance of the Kondo resonance for such parameters and its replacement by the spectra schematically illustrated in Fig. (2d).

Recently, double quantum-dot systems have been fabricated to simulate the two Kondo impurity model [1]. When the two dots are allowed to interact, two split Kondo resonances appear in the tunneling spectra. The spectrum in Fig.(3a) of Ref.[1] is similar to our Fig.(2c), and the two observed peaks can be identified as the even and odd parity resonances of the Kondo dots.

[1] N. J. Craig *et al.*, Science **304**, 565 (2004).
[2] B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B. A. Jones, C. M. Varma, and J. W. Wilkins, *ibid*, **61**, 125(1988); B. A. Jones and C. M. Varma, Phys. Rev. B **40**, 324 (1989).
[3] I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **68**, 1046(1992).
[4] C. Sire, C. M. Varma, and H. R. Krishnamurthy, Phys. Rev. B **48**, 13833(1993).
[5] B. A. Jones, B. G. Kotliar and A. J. Millis, Phys. Rev.

B **39**, 3415 (1989); R. M. Fye, Phys. Rev. Lett. **72**, 916 (1994).
[6] Similar calculations with a different physical emphasis have recently been carried out by G. Zárand *et al.*, cond-mat/0607255.
[7] In terms the local level ϵ_f, Coulomb interaction U, and the hybridization $v_\mathbf{k}$ in the Anderson model, $J_{k,k'} = 2v_k v_{k'}(1/|\epsilon_f| + 1/|\epsilon_f + U|)$ and $V_{k,k'} = (1/2)v_k v_{k'}(1/|\epsilon_f| - 1/|\epsilon_f + U|)$.
[8] We pick $K > 0$ to be antiferromagnetic while $K < 0$ to

be ferromagnetic, while in Ref. [2] another notation I_0 is used with opposite signs.

[9] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[10] D. M. Cragg and P. Lloyd, J. Phys. C: Solid State Phys. **11**, L597 (1978); *ibid*, **12**, 3301(1979).

[11] See, e.g., Th. Pruschke, R. Bulla, and M. Jarrell, Phys. Rev. B **61**, 12799(2000).